Problem statement

We all want to do accurate Bayesian inference quickly:

- In terms of compute (wall time, model evaluations, parallelism)
- In terms of analyst effort (tuning, algorithmic complexity)

Markov Chain Monte Carlo (MCMC) can be straightforward and accurate but slow.

Black Box Variational Inference (BBVI) can be faster alternative to MCMC. **But...**

- BBVI is cast as an optimization problem with an intractable objective ⇒
- Most BBVI methods use **stochastic gradient** (SG) optimization ⇒
    - SG algorithms can be hard to tune
    - Assessing convergence and stochastic error can be difficult
    - SG optimization can perform worse than second-order methods on tractable objectives
- Many BBVI methods employ a **mean-field (MF) approximation** ⇒
    - Posterior variances are poorly estimated

Our proposal: replace the intractable BBVI objective with a fixed approximation.

- Better optimization methods can be used (e.g. true second-order methods)
- Convergence and approximation error can be assessed directly
- Can correct posterior covariances with linear response covariances
- This technique is well-studied (but there's still work to do in the context of BBVI)

⇒ **Simpler, faster, and better BBVI posterior approximations ... in some cases.**

Outline

- BBVI Background and our proposal
  - Automatic differentiation variational inference (ADVI) (a BBVI method)
  - Our approximation: "Deterministic ADVI" (DADVI)
  - Linear response (LR) covariances
  - Estimating approximation error
- Experimental results: DADVI vs ADVI
  - DADVI converges faster than ADVI, and requires no tuning
  - DADVI's posterior mean estimates' accuracy are comparable to ADVI
  - DADVI+LR provides more accurate posterior variance estimates than ADVI
  - DADVI provides accurate estimates of its own approximation error
  - ADVI often results in better objective function values (eventually)
- Why don't we do DADVI all the time?
  - DADVI fails for expressive BBVI approximations (e.g. full-rank ADVI)
  - Pessimistic dimension dependence results from optimization theory
  - ...which may not apply in certain BBVI settings.

Notation

Parameter: $\theta \in \mathbb{R}^{D_\theta}$

Data: y

Prior: $\mathcal{P}(\theta)$ (density w.r.t. Lebesgue $\mathbb{R}^{D_\theta}$, nonzero everywhere)

Likelihood: $\mathcal{P}(y|\theta)$ (nonzero for all θ)

We will be interested in means and covariances of the (intractable) posterior

$$\mathcal{P}(\theta|y) = \frac{\mathcal{P}(\theta, y)}{\int \mathcal{P}(\theta', y)d\theta'}.$$

Denote gradients with ∇, e.g.,

$$\nabla_\theta \log \mathcal{P}(\theta, y) := \left. \frac{\partial \log \mathcal{P}(\theta, y)}{\partial \theta} \right|_\theta \quad \text{and} \quad \nabla_\theta^2 \log \mathcal{P}(\theta, y) := \left. \frac{\partial^2 \log \mathcal{P}(\theta, y)}{\partial \theta \partial \theta^\mathsf{T}} \right|_\theta$$

Assume we have a twice auto-differentiable software implementation of

$$\theta \mapsto \log \mathcal{P}(\theta, y) = \log \mathcal{P}(y|\theta) + \log \mathcal{P}(\theta).$$

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Notation

Automatic differentiation variational inference (ADVI) is a particular BBVI method.

ADVI specifies a family $\Omega_{\mathcal{Q}}$ of D_θ-dimensional Gaussian distributions.

The family $\Omega_{\mathcal{Q}}$ is parameterized by $\eta \in \mathbb{R}^{D_\eta}$, encoding the means and covariances.

The covariances of the family $\Omega_{\mathcal{Q}}$ can either be

- Diagonal: "Mean-field" (MF) approximation, $D_\eta = 2D_\theta$
- Any PD matrix: "Full-rank" (FR) approximation, $D_\eta = D_\theta + D_\theta(D_\theta - 1)/2$

$$\underset{\mathcal{Q} \in \Omega_{\mathcal{Q}}}{\operatorname{argmin}} \operatorname{KL}\left(\mathcal{Q}(\theta|\eta)||\mathcal{P}(\theta|y)\right) = \underset{\eta \in \mathbb{R}^{D_\eta}}{\operatorname{argmin}} \operatorname{KL}_{\mathrm{VI}}(\eta)$$

$$\text{where } \operatorname{KL}_{\mathrm{VI}}(\eta) := \underset{\mathcal{Q}(\theta|\eta)}{\mathbb{E}}\left[\log \mathcal{Q}(\theta|\eta)\right] - \underset{\mathcal{Q}(\theta|\eta)}{\mathbb{E}}\left[\log \mathcal{P}(\theta, y)\right]$$

$$= \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}}\left[\log \mathcal{Q}(\theta(z, \eta)|\eta)\right] - \underbrace{\underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}}\left[\log \mathcal{P}(\theta(z, \eta), y)\right]}_{\text{Typically intractable}}.$$

The final line uses the "reparameterization trick" with standard Gaussian $z \sim \mathcal{N}_{\mathrm{std}}(z)$.

ADVI is an instance of the general problem of finding

$$\underset{\eta}{\operatorname{argmin}} F(\eta) \text{ where } F(\eta) := \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}}\left[f(\eta, z)\right].$$

Two approaches

Consider $\quad \underset{\eta}{\text{argmin}}\, F(\eta) \quad$ where $\quad F(\eta) := \underset{\mathcal{N}_{\text{std}}(z)}{\mathbb{E}}\left[f(\eta, z)\right].$

Let $\mathcal{Z}_N = \{z_1, \ldots, z_N\} \overset{iid}{\sim} \mathcal{N}_{\text{std}}(z)$, and let $\hat{F}(\eta|\mathcal{Z}_N) := \frac{1}{N}\sum_{n=1}^{N} f(\eta, z_n)$.

Algorithm 1	**Algorithm 2**
Stochastic gradient (SG)	Sample average approximation (SAA)
ADVI (and most BBVI)	Deterministic ADVI (DADVI) (proposal)

Algorithm 1

Fix N (typically $N = 1$)
$t \leftarrow 0$
while Not converged **do**
$\quad t \leftarrow t + 1$
$\quad$ Draw $\mathcal{Z}_N$
$\quad \Delta_S \leftarrow \nabla_\eta \hat{F}(\eta_{t-1}|\mathcal{Z}_N)$
$\quad \alpha_t \leftarrow \text{SetStepSize}(\text{Past state})$
$\quad \eta_t \leftarrow \eta_{t-1} - \alpha_t \Delta_S$
$\quad \text{AssessConvergence}(\text{Past state})$
end while
return η_t or $\frac{1}{M}\sum_{t'=t-M}^{t} \eta_{t'}$

Algorithm 2

Fix N (our experiments use $N = 30$)
Draw $\mathcal{Z}_N$
$t \leftarrow 0$
while Not converged **do**
$\quad t \leftarrow t + 1$
$\quad \Delta_D \leftarrow \text{GetStep}(\hat{F}(\cdot|\mathcal{Z}_N), \eta_{t-1})$
$\quad \eta_t \leftarrow \eta_{t-1} + \Delta_D$
$\quad \text{AssessConvergence}(\hat{F}(\cdot|\mathcal{Z}_N), \eta_t)$
end while
return η_t

Our proposal: Apply algorithm 2 with the ADVI objective.
Take better steps, easily assess convergence, with less tuning.

Experiments

For each of a range of models (next slide), we compared:

- **NUTS:** The "no-U-turn" MCMC sampler as implemented by PyMC [Salvatier et al., 2016]. We used this as the "ground truth" posterior.

- **DADVI:** We used $N = 30$ draws for DADVI for each model. We optimized using an off-the-shelf second-order Newton trust region method (`trust-ncg` in `scipy.optimize.minimize`) with no tuning or preconditioning.

  Stochastic ADVI methods:

- Mean field ADVI: We used the PyMC implementation of ADVI, together with its default termination criterion (based on parameter differences).
- Full-rank ADVI: We used the PyMC implementation of full-rank ADVI, together with the default termination criterion for ADVI described above.
- RAABBVI: To run RAABBVI, we used the public package `viabel`, provided by Welandawe et al. [2022].
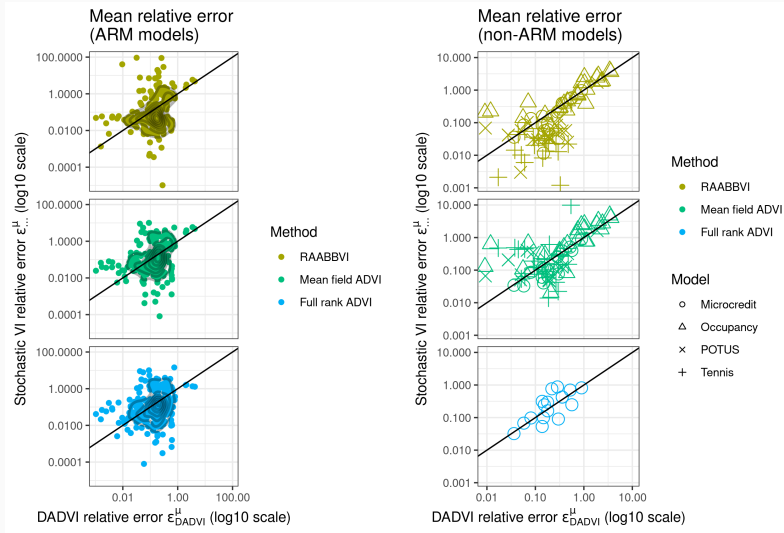
We terminated unconverged stochastic ADVI after 100,000 iterations.

Experiments

We evaluated DADVI on a range of models.

| Model Name	Dim D_θ	NUTS runtime	Description
ARM (53 models)	Median 5 (max 176)	median 39 seconds (max 16 minutes)	A range of linear models, GLMs, and GLMMs
Microcredit	124	597 minutes	Hierarchical model with heavy tails and zero inflation
Occupancy	1,884	251 minutes	Binary regression with highly crossed random effects
Tennis	5,014	57 minutes	Binary regression with highly crossed random effects
POTUS	15,098	643 minutes	Autoregressive time series with random effects

Table 1: Model summaries.

Figure 1: Posterior mean accuracy (relative to MCMC posterior standard deviation). Each point is a single named parameter in a single model. Points above the diagonal line indicate better DADVI or LRVB performance.
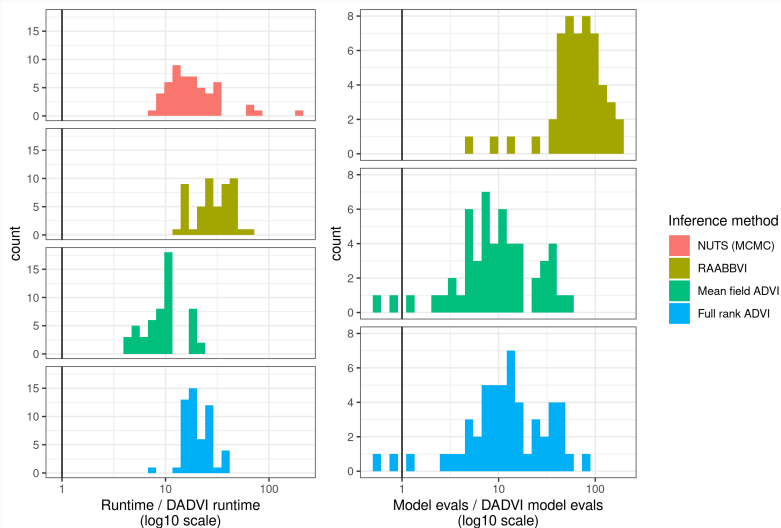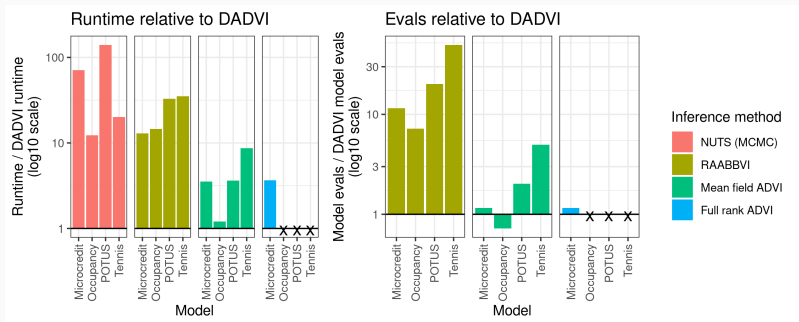
Figure 2: Runtimes and model evaluation counts for the ARM models. Results are reported divided by the corresponding value for DADVI.
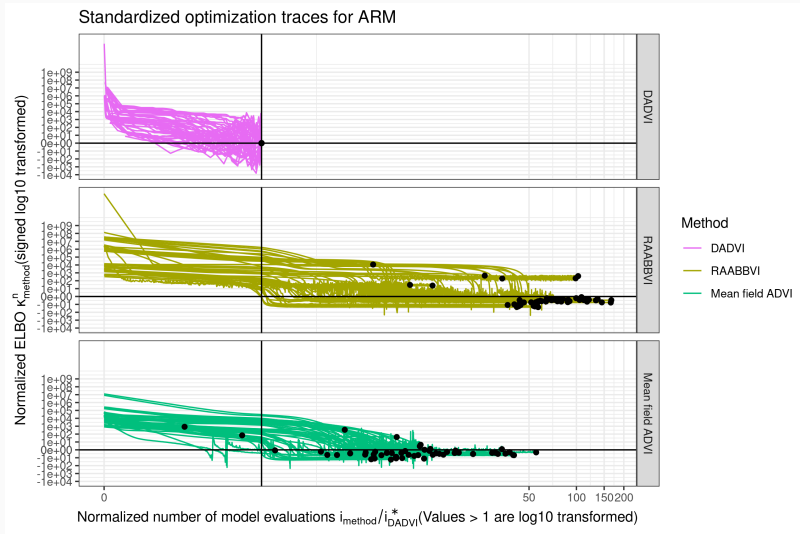
Figure 3: Runtimes and model evaluation counts for the non-ARM models. Results are reported divided by the corresponding value for DADVI. Missing model / method combinations are marked with an X.

Figure 4: Optimization traces for the ARM models. Black dots show the termination point of each method. Dots above the horizontal black line mean that DADVI found a better ELBO. Dots to the right of the black line mean that DADVI terminated sooner in terms of model evaluations.

Optimization traces for non-ARM models
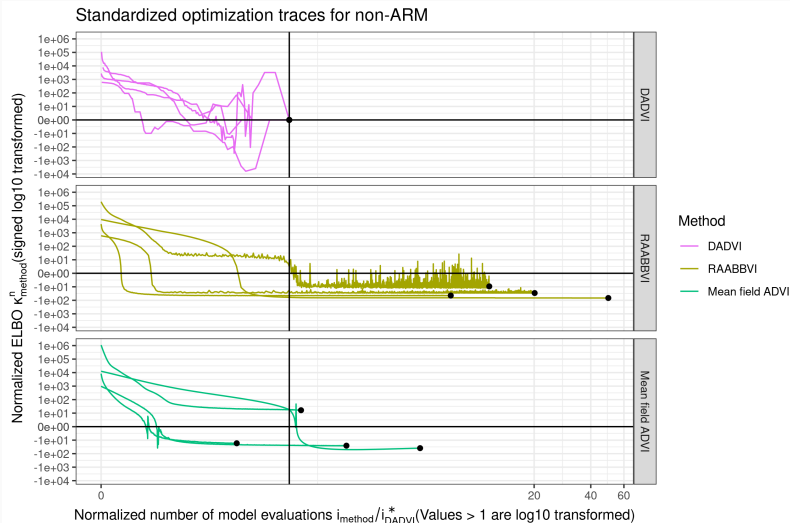
Figure 5: Traces for non-ARM models. Black dots show the termination point of each method. Dots above the horizontal black line mean that DADVI found a better ELBO. Dots to the right of the black line mean that DADVI terminated sooner in terms of model evaluations.

Linear response covariances and sampling uncertainty

Intractable objective:

$$\overset{*}{\eta} = \underset{\eta \in \mathbb{R}^{D_\eta}}{\operatorname{argmin}} \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}} [f(\eta, z)]$$

DADVI approximation:

$$\hat{\eta}(\mathcal{Z}_N) = \underset{\eta \in \mathbb{R}^{D_\eta}}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} f(\eta, z_n).$$

What is the error of the DADVI approximation $\hat{\eta} - \overset{*}{\eta}$?

$\Leftrightarrow$ What is the distribution of the DADVI error $\hat{\eta} - \overset{*}{\eta}$ under sampling of $\mathcal{Z}_N$?

Answer: The same as a that of any M-estimator: asymptotically normal (as N grows)

Posterior variances are often badly estimated by mean-field (MF) approximations.

Linear response (LR) covariances improve covariance estimates by computing *sensitivity* of the variational means to particular perturbations. [Giordano et al., 2018]
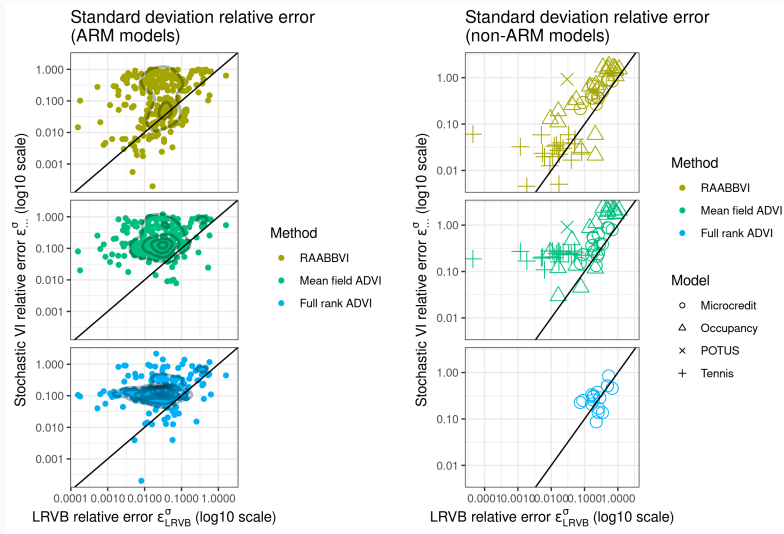
Example: With a correlated Gaussian $\mathcal{P}(\theta|y)$, the ADVI means are exactly correct, the ADVI variances are underestimated, and LR covariances are exactly correct.

Both DADVI error and LR covariances can be computed using $\nabla^2_\eta \, \widehat{\mathrm{KL}}_{\mathrm{VI}}(\hat{\eta})$.
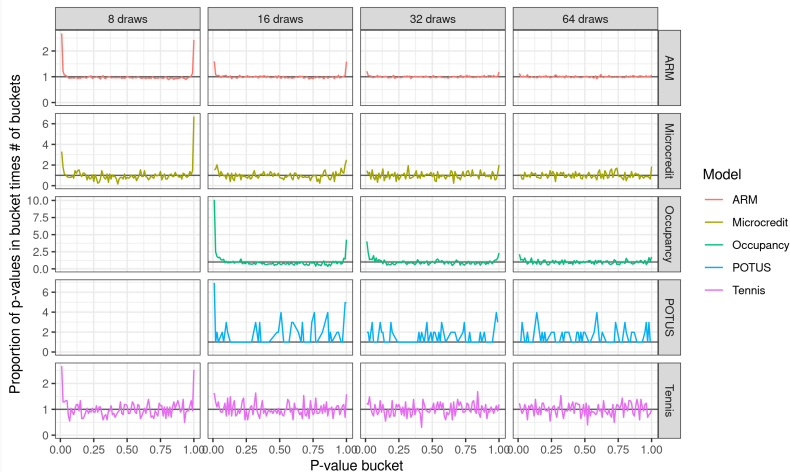
Stochastic ADVI does not produce an actual optimum of any tractable objective, so LR and M-estimator computations are unavailable.

Figure 6: Posterior sd relative accuracy. Each point is a single named parameter in a single model. Points above the diagonal line indicate better DADVI or LRVB performance.

DADVI approximation error accuracy

Figure 7: Density estimates of $\Phi(\varepsilon^\xi)$ for difference models. All the ARM models are grouped together for ease of visualization. Each panel shows a binned estimate of the density of $\Phi(\varepsilon^\xi)$ for a particular model and number of draws N. Values close to one (a uniform density) indicate good frequentist performance. CG failed for the Occupancy and POTUS models with only 8 draws, possibly indicating poor optimization performance with so few samples.

Previous theoretical results

Intractable objective:

$$\check{\eta} = \operatorname*{argmin}_{\eta \in \mathbb{R}^{D_\eta}} \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}} [f(\eta, z)]$$

SAA approximation (DADVI):

$$\hat{\eta}(\mathcal{Z}_N) = \operatorname*{argmin}_{\eta \in \mathbb{R}^{D_\eta}} \frac{1}{N} \sum_{n=1}^{N} f(\eta, z_n).$$

The idea of optimizing $\hat{F}$ instead of SG on F is old and well-studied in the optimization literature, where $\hat{F}$ is known as the **Sample average approximation (SAA)**.

Yet SAA is rarely used for BBVI.[1] One possible reason is the following:

Theorem [Nemirovski et al., 2009]: In general, the error of both SG and SAA scale as $\sqrt{D_\theta/N}$, where, for SG, N is the *total number of samples used*.

- For SG, each z_n gets used once (for a single gradient step)
- For SAA, each z_n gets used once per optimization step (of which the are many).
- Often, in higher dimensions, SAA requires more optimization steps.

Corollary: [Kim et al., 2015] In general, for a given accuracy, the computation required for SAA scales worse than SG as the dimension D_θ grows.

We got good results with D_θ as high as $15,098$ using only only $N = 30$. Why?

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[1]Some exceptions I'm aware of: Giordano et al. [2018, 2022], Wycoff et al. [2022], Burroni et al. [2023].

Some first steps

Theorem [Giordano et al., 2023]: When $\mathcal{P}(\theta|y)$ is multivariate normal, and we use the mean-field Gaussian approximation, then, for any particular entry η_d of η, then $\left| \hat{\eta}_d - \mathring{\eta}_d \right| = O_p(N^{-1/2})$ irrespective of D_θ.

Theorem [Giordano et al., 2023]: Assume $\mathcal{P}(\theta|y)$ has a "global-local" structure:

$$\theta = (\gamma, \lambda_1, \ldots, \lambda_{D_\lambda}) \qquad \mathcal{P}(\gamma, \lambda_1, \ldots, \lambda_{D_\lambda}|y) = \prod_{d=1}^{D_\lambda} \mathcal{P}(\gamma, \lambda_d|y).$$

Assume that the dimension of γ and each λ_d stays fixed as D_λ grows.

Under regularity conditions, the DADVI error scales as $\sqrt{\log D_\lambda / N}$, not $\sqrt{D_\lambda / N}$.

Proposal: The "in general" analysis of [Nemirovski et al., 2009] is too general for many practically interesting BBVI problems.

A negative result

Theorem [Giordano et al., 2023]: Assume that $N < D_\theta$, and that we use a full-rank Gaussian approximation. Then the DADVI objective is unbounded below, and optimization of the DADVI objective will approach a degenerate point mass at $\mathrm{argmax}_\theta \log \mathcal{P}(\theta|y)$.

Proof sketch: For any value of the variational mean, the DADVI objective only depends on $\mathcal{P}(\theta|y)$ evaluated in a subspace spanned by $\mathcal{Z}_N$. The variational objective can be driven to $-\infty$ by driving the variance to zero in the subspace orthogonal to $\mathcal{Z}_N$.

Proposal: All sufficiently expressive variational approximations (e.g. normalizing flows) will fail in the same way in high dimensions. However, this pathology can be obscured and overlooked in practice by low-quality optimization.

Conclusion

Black Box Variational Inference with a Deterministic Objective: Faster, More Accurate, and Even More Black Box.

Giordano, R.*, Ingram, M.*, Broderick, T. (* joint first authors), 2023.

(Arxiv preprint here.)

- By fixing the randomness in the ADVI objective, DADVI provides BBVI that is easier to use, faster, and more accurate than stochastic gradient.
- The approximation used by DADVI will not work in high dimensions for sufficiently expressive approximating distributions (e.g., full-rank ADVI).
- There appears to be a gap between the optimization literature and BBVI practice in high dimensions for a class of practically interesting problems.

References

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Supplemental material

Linear response covariances

Posterior variances are often badly estimated by mean-field (MF) approximations.

Example: With a correlated Gaussian $\mathcal{P}(\theta|y)$ with ADVI, the ADVI means are correct, but the ADVI variances are underestimated.

Take a variational approximation $\mathring{\eta} := \operatorname{argmin}_{\eta \in \mathbb{R}^{D_\eta}} \operatorname{KL}_{\mathrm{VI}}(\eta)$. Often,

$$\underset{\mathcal{Q}(\theta|\mathring{\eta})}{\mathbb{E}}[\theta] \approx \underset{\mathcal{P}(\theta|y)}{\mathbb{E}}[\theta] \quad \text{but} \quad \underset{\mathcal{Q}(\theta|\mathring{\eta})}{\operatorname{Var}}(\theta) \neq \underset{\mathcal{P}(\theta|y)}{\operatorname{Var}}(\theta). \tag{1}$$

Example: Correlated Gaussian $\mathcal{P}(\theta|y)$ with ADVI.

Linear response covariances use the fact that, if $\mathcal{P}(\theta|y,t) \propto \mathcal{P}(\theta|y)\exp(t\theta)$, then

$$\left.\frac{d \underset{\mathcal{P}(\theta|y,t)}{\mathbb{E}}[\theta]}{dt}\right|_{t=0} = \underset{\mathcal{P}(\theta|y)}{\operatorname{Cov}}(\theta). \tag{2}$$

Let $\mathring{\eta}(t)$ be the variational approximation to $\mathcal{P}(\theta|y,t)$, and take

$$\underset{\mathcal{Q}(\theta|\mathring{\eta})}{\operatorname{LRCov}}(\theta) = \left.\frac{d \underset{\mathcal{Q}(\theta|\mathring{\eta}(t))}{\mathbb{E}}[\theta]}{dt}\right|_{t=0} = \left(\nabla_\eta \underset{\mathcal{Q}(\theta|\mathring{\eta})}{\mathbb{E}}[\theta]\right)\left(\nabla_\eta^2 \operatorname{KL}_{\mathrm{VI}}(\mathring{\eta})\right)^{-1}\left(\nabla_\eta \underset{\mathcal{Q}(\theta|\mathring{\eta})}{\mathbb{E}}[\theta]\right)$$

Example: For ADVI with a correlated Gaussian $\mathcal{P}(\theta|y)$, $\underset{\mathcal{Q}(\theta|\mathring{\eta})}{\operatorname{LRCov}}(\theta) = \underset{\mathcal{Q}(\theta|\mathring{\eta})}{\operatorname{Cov}}(\theta)$.